

Bioaccumulation Equation Q

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Kinetic Bioaccumulation Equation

(Arnot & Gobas 2004)

$$\frac{dM_B}{dt} = \left\{ W_B \cdot \left(k_1 \cdot [m_O \cdot C_{WD,O} + m_P \cdot C_{WD,P}] + k_D \cdot \sum_i (P_i \cdot C_{D,i}) \right) \right\} - (k_2 + k_E + k_M) \cdot M_B + k_G$$

- M_B = mass of chemical in organism (g)
- W_B = weight of organism (kg)
- k_1 = gill uptake from water m_o or pore water m_p (g/ kg·d)
- $k_D \sum()$ = uptake from diet summed over dietary preferences (g/ kg·d)
- k_2 = gill depuration (1/d)
- k_E = fecal elimination (1/d)
- k_M = metabolism (1/d)
- k_G = growth dilution -- *explicitly added unless dynamically modeling weight of organism over time*

Transform Equation

$$\frac{dM_B}{dt} = \left\{ W_B \cdot \left(k_1 \cdot [m_O \cdot C_{WD,O} + m_P \cdot C_{WD,P}] + k_D \cdot \sum_i (P_i \cdot C_{D,i}) \right) \right\} - (k_2 + k_E + k_M + k_G) \cdot M_B$$

- Code calculates concentration in organism
 M_B/W_B
- Divide each side by W_B
- Multiply each side by DT
- $(M_B/W_B)_{T1} = (M_B/W_B)_{T0} + DT(K1[] + K_D \sum()) - DT (M_B/W_B)_{T0} (K_2 + K_E + K_M + K_G)$

R Code

Current Code:

```
# Calculate tissue concentration

CB[iTS, OrgNames_a[iOrg], iArea, iChem, iSeg, iRemed] =
(CBi[iOrg] + (DT * (K1_ac[iOrg] * ((1 - FPW[iOrg]) * CWB_acst + FPW[iOrg] * CSD_acst) + KD_ac[iOrg] * sum_C_DF_oac))) /
(1 + DT * (K2_ac[iOrg] + KE_ac[iOrg] + KG_a[iOrg] + KM_c[iOrg]))
```

Suggest it should be

```
# Calculate tissue concentration

CB[iTS, OrgNames_a[iOrg], iArea, iChem, iSeg, iRemed] =
(CBi[iOrg] +
((DT * (K1_ac[iOrg] * ((1 - FPW[iOrg]) * CWB_acst + FPW[iOrg] * CSD_acst) + KD_ac[iOrg] * sum_C_DF_oac)) -
(DT * CBi[iOrg]*(K2_ac[iOrg] + KE_ac[iOrg] + KG_a[iOrg] + KM_c[iOrg]))))
```